ERDC MSRC/PET TR/00-21

Contract Year Five

Programming Environment and Training (PET)

Core Support and Focused Efforts

for

U.S. Army Engineer Research and Development Center (ERDC)

Major Shared Resource Center (MSRC)

06h00102000

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for ERDC MSRC

1. Introduction

2. Year Five Efforts

3. Contact Information

Section 1: INTRODUCTION

1.1 BACKGROUND

As a result of the Annual Review for the U.S. Army Engineer Research and Development Center (ERDC) Major Shared Resource Center (MSRC) Programming Environment and Training (PET) program that occurred on 15-16 February 2000, a follow-on series of Core Support and Focused Efforts have been endorsed. These cover the primary Computational Technology Areas (CTAs) supported by the center and other specialty areas, including Scientific Visualization (SV), Scalable Parallel Programming (SPP) Tools, support for Historically Black Colleges and Universities (HBCUs) and Minority Institutions (MIs), Training, and Collaboration/Communication (C/C). The primary CTAs supported at ERDC MSRC are Computational Fluid Dynamics (CFD), Computational Structural Mechanics (CSM), Environmental Quality Modeling and Simulation (EQM), Climate/Weather/Ocean Modeling and Simulation (CWO), and Forces Modeling and Simulation/C4I (FMS).

The academic partners associated with ERDC MSRC PET include: Engineering Research Center (ERC) at Mississippi State University (Lead University); Jackson State University (HBCU/MI Lead); National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign; Rice University; University of Tennessee, Knoxville; Florida State University; Clark Atlanta University (HBCU); Ohio Supercomputing Center; Ohio State University; Texas Institute for Computational and Applied Mathematics (TICAM) at the University of Texas at Austin; Texas A&M University – Kingsville (MI).

1.2 CORE SUPPORT

"Core Support" refers to that portion of PET that captures the minimum funding required for full-time on-site positions and university leads. Significant lead time and funding assurance are required prior to university hiring commitments, so there must be some level of assurance that annual funding will be maintained at each university throughout the program. This, of course, does not preclude corrective action based on non-performance. PET activities at ERDC MSRC within Core Support include, but are not limited to:

- Providing High Performance Computing (HPC) training courses for MSRC users
- Providing a continual base of academic involvement in PET
- Ensuring greater freedom in the scope of university efforts
- Providing for longer duration academic efforts
- User outreach based on constant CTA utilization monitoring, DoD HPC User Group Conference participation, and one-on-one user assistance as required
- Providing updated inputs to PET web pages
- Regular reporting of activities/progress for each PET area

- SPP algorithm enhancement
- PET support role in computational migration

The following Core Support efforts were approved for Year Five:

Jackson State University
- HPC Support to HBCU/MIs, Off-site

Florida State University
- Communication/Collaboration (C/C), Off-site
- Training, Off-site

Mississippi State University
- Academic Lead, Off-site
- Computational Fluid Dynamics (CFD), On-site and Off-site
- Computational Structural Mechanics (CSM), On-site

Ohio State University
- Climate/Weather/Ocean Modeling and Simulation (CWO), On-site and Off-site

Rice University
- Scalable Parallel Programming Tools, On-site and Off-site

University of Texas at Austin
- Environmental Quality Modeling and Simulation (EQM), On-site and Off-site
- Computational Structural Mechanics (CSM), Off-site

1.3 FOCUSED EFFORTS

"Focused Efforts" are activities funded by the additional PET resources, which are allocated for approved projects based on PET team interactions with MSRC users and on proposals submitted by the university partners and approved by the PET leadership and ERDC MSRC. Focused Effort proposals are evaluated according to the following guidelines:

- Each proposed effort should be an HPC support activity related to national defense or national security.
- Relevance of proposed activity to ongoing Common HPC Software Support Initiative (CHSSI) projects is considered.
- Extent to which the proposed effort complements MSRC hardware acquisition strategy is considered.
- Proposed effort relevance to ongoing DoD Challenge Projects is considered.
- Proposed effort exploitation of the Defense Research and Engineering Network (DREN) network capabilities is considered.

- Efforts should improve the effective utilization of HPC resources via
  - Visualization and data interpretation
  - Code performance enhancements
  - Multi-architecture portability, etc.
- Proposed efforts should enhance the capability to use MSRC systems via
  - Training and graduate courses
  - HBCU/MI activities
  - Collaborative environments, etc.

Obviously, every Focused Effort cannot meet all of these criteria. These criteria are used to judge the importance of the proposed work with respect to the HPCMP mission. Focused Efforts are managed according to the following rules:

- Authority to Proceed (ATP) is based on informal proposals submitted to the PET Director and the review/concurrence of PET leadership and the government.
- Projects must have MSRC user advocacy and participation if at all possible.
- Projects should have specific start and end dates, schedules, work products, budgets, and periodic progress reviews (every 3 months).
- Each effort is managed on a project-by-project basis, and funding will be allocated on this basis.
- Final technical reports are due at the end of the contract year.

The following Focused Efforts have been approved for Year Five:

Clark Atlanta University

- Development of Web-based Training Material on ERDC MSRC HPC Systems (Student Internship)
- Parallel Simulation of Wave Break and Waves Interacting with Vessels in Motion

Florida State University

- Modular Collaborative Environment
- Collaborative Computational Portals for Training and Science
- Ubiquitous Access to HPC Resources
- Computational Science and Information Technology: Curriculum and Technology

University of Illinois at Urbana-Champaign

- Standard File Format for Large Data Problems and Visualization

Mississippi State University

- Grid Assembly Enhancements for Chimera Technology
- Java Based CFD Training
- Library of Interpolation and Approximation Modules (INLiB)

Ohio State University

- Enhancement, Evaluation, and Application of a Coupled Wave -Current-Sediment Model for Nearshore and Tributary Plume Predictions

Ohio Supercomputer Center

- HPC Training Courses

University of Tennessee, Knoxville

- Parallel IO
- Metacomputing Support for the SARA3D Structural Technology Acoustics Application

University of Texas at Austin

- AMR and CTH Capability and Algorithm Enhancements
- Adaptive Mesh Technology, Mesh Improvement and Algorithms for Hypervel ocity Impact and Penetration Analyses
- Discontinuous Galerkin Finite Elements and Adaptive Grids for DoD Problems
- Algorithms for Error and Feature Indication in Interpolation and Approximation
- Improved Parallel Performance for Environmental Quality Models
- A Full 2-D Parallel Implementation of CH3D-Z
- Interpolation and Projection Between Arbitrary Space/Time Grids
- Reactive Transport Schemes for Water Quality Modeling on Unstructured Grids

Texas A&M University – Kingsville

- Parallel FEMWATER Visualization
- Parallel FEMWATER Data Management

Detailed descriptions of the approved Year Five Core Support and Focused Efforts are provided in Section 2.

The overall working theme for ERDC MSRC is “Scalable HPC Applications and Performance.” Within this context PET is supporting a number of thematic areas, including Scalable Computing Migration, HPC Training and DoD User Productivity, HPC Performance Metrics/Tools, Management and Interpretations of Large Data Sets, SciVis for Very Large (Terabyte Scale) Problems, and D oD Challenge Applications. The PET Core Support and Focused Efforts support the overall ERDC MSRC theme and thematic areas.

Section 2

ERDC MSRC PET
YEAR FIVE CORE SUPPORT
and
FOCUSED EFFORTS

1. **Focused Effort Title:** Development of Web-based Training Material on ERDC MSRC HPC Systems (Student Internship)

2. **Organization:** Clark Atlanta University

3. **Thematic Area:** HPC Training and DoD User Productivity

4. **PI Name:** Prof. Kofi Bota

5. **E-Mail:** kbota@cau.edu

6. **Telephone:** (404) 880-6996

7. **Fax:** (404) 880-6880

8. **Statement of Work:**

   Clark Atlanta University will provide a student to work on -site at ERDC MSRC during the months of June, July, and August 2000. The student will assist in the development of ERDC MSRC web pages to provide users information on the ERDC MSRC HPC computer systems. For example, this could include information on using PBS, compiling and executing programs, migrating data, and resources (hardware and software) available on the various systems.

   Assumption: All equipment, material, and information will be supplied by ERDC MSRC.

9. **Deliverables:**

   - Web pages for ERDC MSRC Webmaster
   - Presentation and Final Report

1. **Focused Effort Title:** Parallel Simulation of Wave Break and Waves Inter acting with Vessels in Motion

2. **Organization:** Clark Atlanta University

3. **Thematic Areas:** Scalable Computing Migration, HPC Performance Metrics/Tools

4. **PI Name:** Prof. Shahrouz Aliabadi

5. **E-Mail:** aliabadi@cau.edu

6. **Telephone:** (404) 880-6433

7. **Fax:** (404) 880-6880

8. **Statement of Work:**

In coastal wave modeling, the wave energy balance equation is solved in terms of wave spectra. Waves break in relatively shallow water or in areas where they steepen on currents. There has been little work done on modeling the wave breaking from first principles. The dissipation source terms applied in wave models are empirical and derived from field and lab measurements. Having a computer modeling of wave break capability would allow us to derive more accur ate dissipation functions, as well as gain insight on the physics of specific problems. This valuable information is extremely difficult, costly and in some cases impossible to obtain through measurements in laboratories. Dr. Jane Smith from the ERDC Coastal and Hydraulic Laboratory (ERDC CHL) has interest in numerical simulations of wave break to study the energy dissipation, wave height and structure, nonlinear energy transfers and turbulent fluctuations.

Drs. Charlie Berger and Jane Smith also from ERD C CHL would like to study flow behavior underneath ships in motion and waves interacting with vessels in motion. It is extremely difficult to carry out full -scale experiments to measure flow properties and characteristics for such problems. In these cases, computer modeling can be used as an alternative tool to study flow behavior.

During the past several years, we have developed highly scalable parallel finite element flow solvers for simulation of multi -fluid flow applications. Our solvers are based on t he Navier–Stokes equations for multiple incompressible fluids mixing with each other. Stabilized finite element formulations are used for the discretization of the governing equations. The non -linear systems of equations resulting from the finite element discretizations are solved using sophisticated vector -based iterative solvers. As a result, minimal memory is required to solve applications with 10 to 100 million unknowns. The parallel implementation of the solver assumes that the finite element mesh is t otally unstructured. This greatly broadens the application of the solver to problems with complex geometries discretized with automatic mesh generators. The parallel implementation is also based on the MPI, which makes the solver portable to any supercompu ter platform. Currently we are running our solver on the Cray T3E, IBM SP2 and SGI Power Challenge. Recently, the accuracy of this flow solver has been verified in 3D applications.

In this project, we will apply our parallel finite element flow solver to simulate breaking wave problems. We will investigate the structure of wave formation and wave break in a computer environment resembling the physical condition. We will also apply our flow solver to simulate waves interacting with vessels in motion. This project will be conducted through extensive collaborations and discussions with Drs. Charlie Berger and Jane Smith from the ERDC CHL.

9. Deliverables:

- Simulation of wave formation and wave breaking problems. This includes geometry modeling, mesh generation, parallel computation, flow visualization and interpreting the results.
- Simulation of waves interacting with ships in motion. We will create an unstructured mesh for a complex 3D ship geometry and its domain of computation. Parallel simulations will be carried out on a Cray T3E.
- Multiple meetings with Drs. Charlie Berger and Jane Smith to discuss the results and future trends. These meeting will be held either at ERDC or Clark Atlanta University.
- We will leverage this project to train undergraduate students in parallel computation and HPC.
- Presenting the results in conferences or workshops
- Trip Reports
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Core Support Area:** Communication/Collaboration (C/C)
2. **Organization:** Florida State University
3. **Lead:** Prof. Geoffrey Fox
4. **E-Mail:** gcf@cs.fsu.edu
5. **Telephone:** (850) 644-4587
6. **Fax:** (850) 644-0098
7. **Statement of Work:**

Florida State will provide a core level of effort to support technology transfer, user outreach, training, and assessment of tools and technologies to facilitate communication and collaboration among the PET team and users of the ERDC MSRC. Technologies of interest include, but are not limited to, both synchronous and asynchronous collaboration over the Internet and use of databases to manage large volumes of information, especially when coupled with web servers to facilitate access to the information. As a new area of interest, we propose adding handheld devices to this core support effort.

Since the TangoInteractive collaboratory tool has been commercialized through the company WebWisdom.com, Florida State does not plan to provide technical support or further enhancements to the core system. However we will continue to use Tango Interactive and will assist PET partners with its use. Florida State will continue to operate and enhance web-linked database applications Syracuse developed for ERDC MSRC, and, as requested, assist with transfer to on-site computer systems.

Florida State will maintain frequent contact with ERDC MSRC Webmaster, database administrators, and other on-site personnel to insure that C/C resources provide the maximum utility to the PET/user community. Florida State will also maintain regular contact with PET team members to assess needs. Florida State will select and attend focused conferences and other meetings that have high payoff and direct application for team and user interaction and technology transfer.

Handheld Core Effort: Handheld/wearable digital devices, and the associated wireless communications infrastructures, are a rapidly growing and very interesting area of computing technology. With the potential to link to the Internet and the Grid, as well as to specialized sensors and instrumentation, these tools create many new opportunities. Although we will propose focused efforts for specific projects in this area, it has become clear that a general technology tracking effort is necessary in order to help understand the capabilities of the numerous new devices which are appearing on the market, the role of industry efforts such as WAP (wireless application protocol) and Bluetooth, and the general directions of the market. This will give us a better capability to take advantage of "commodity" devices and standards, while also helping to understand where they might not meet the needs of "handheld high performance computing" (hHPC), which is in many respects NOT a commodity application of these devices. As part of this tracking effort, we will:

1. Follow, and at appropriate times, analyze industry standards/initiatives (i.e. WAP, Bluetooth) in the context of hHPC
2. Track the actual availability of new devices and new capabilities which may be important for hHPC
3. Where appropriate, acquire and analyze devices to obtain a more detailed understanding of their potential in hHPC
4. Maintain a web site at FSU where the results of this tracking will be made available
5. We also propose to organize a workshop at FSU "Hand-Held Supercomputing" which will bring together representatives of industry, academia, and HPC communities.

Collaboration Core Effort: Our strategy is similar to that for training; namely to combine a user requirement analysis, lessons from the previous work and a survey of available tools where we will concentrate on a modules including audio - video conferencing, shared presentation and editing and brainstorming tools. We will include "inhouse" technology (TangoInteractive) as well as other commercial and academic efforts. In the critical audio - video conferencing arena we will include BuenaVista (From TangoInteractive), CUSeeMe, Access Grid (Argonne/NCSA), NetMeeting and the emerging Internet Phones. The analysis will be in the architectural context of a "Collaborative Portal"

We will use our past experience (where TangoInteractive only had limited acceptance outside training) to design a requirements analysis covering training, computer users and MSRC staff. We will present preliminary reports at midyear and use these to design some experimental deployment efforts in the last half of the year.

8. Deliverables:

- Trip reports for conferences and user contacts (as appropriate)
- Contribute materials pertaining to collaboration and communication technologies to the ERDC MSRC PET C/C web site (on-going)
- Report on selected collaboration tools and their possible roles within the ERDC MSRC and PET organizations
- Selected experimental deployment of identified collaboration tools
- Report on selected handheld devices and their role in training and high performance computing.
- Tutorial on Handheld devices
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews

1. **Core Support Area:** Training
2. **Organization:** Florida State University
3. **Lead:** Prof. Geoffrey Fox
4. **E-Mail:** gcf@cs.fsu.edu
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6. **Fax:** (850) 644-0098
7. **Statement of Work:**

Core Technology Tracking and Transfer: Florida State will provide a core level of effort to support technology transfe r, user outreach, and long -range leadership on issues of technology, tools, and techniques related to PET Training and Educational needs. Technologies of interest include, but are not limited to, synchronous and asynchronous web/Internet-based distance edu cation tools, electronic repositories of training materials, etc.

Florida State will work closely with the on -site Training team at the ERDC MSRC to understand the needs and use of training technology at the MSRC in the context of the changing technology base. This requirement analysis will be complemented by a survey of current and emerging tools which we will classify in terms of the concept of a "collaborative portal" which will underlie our research efforts at Florida State and capture the lessons from the PET and other efforts funded at Syracuse over the last few years. A technology of clear importance is XML to either describe Mathematics or Graphics or to define the overall component structure of a portal. We will recommend tools and standards that will enable authoring of training material that can best be re -used as the underlying technology base shifts. We will complete an initial survey by the mid -year review and document with reports and presentations. We will select and support some key tools f or user experimentation and evaluation in the second half of year 5.

Florida State will continue to select and attend focused conferences and other meetings that have high payoff and contribute directly to providing leadership on training technology issues. We expect this effort to position the MSRC to be able to make innovative use of emerging training technology and standards and continue its leadership position in year 6 and beyond.

User Outreach: We will conduct a specialized requirements analysis ba sing survey on capabilities of common tools such as Syracuse's VPL (Virtual Programming Laboratory) for computing instruction, WebCT and PowerPoint for authoring, TangoInteractive for synchronous Instruction, Blackboard for database support. We will analyz e these in the collaborative portal concept using common Web Information Portals as an initial motivator. We will cover both MSRC and HBCU users.

Training: As part of our effort to support the use of distance training tools within the PET program, we plan to offer a Distance Training Workshop covering approaches for both synchronous and asynchronous modes of delivery. We will include a tutorial on base

technologies, especially XML, covering the use of the Object web in all areas of relevance to the MSRC. We will include those tools selected as part of our mid-year report.

8. Deliverables:

- Trip reports for conferences and user contacts
- Contribute materials pertaining to education and training technologies to the ERDC MRSC PET Training web site (on-going)
- Involvement in PET Program-Wide Training Group meetings and activities
- Report evaluating training and education tools linked to both MSRC user and HBCU pipeline requirements
- Support of selected tools such as XML Portal construction and database systems as well as VPL (or better) programming interface.
- Hosting of TangoInteractive Servers as needed by MSRC training and education
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Revie ws

ERDC MSRC PET YEAR FIVE EFFORTS

1. **Focused Effort Title:** Modular Collaborative Environment
2. **Organization:** Florida State University
3. **Thematic Area:** HPC Training and DoD User Productivity
4. **PI Names:** Dr. David Bernholdt, Prof. Geoffrey Fox
5. **E-Mail:** bernhold@npac.syr.edu , gcf@cs.fsu.edu
6. **Telephone:** (315) 443-3857, (850) 644-4587
7. **Fax:** (315) 443-1943, (850) 644-0098
8. **Statement of Work:**

   As part of this effort, we intend to look again at commercial desktop conferencing. We intend to install and test the Access Grid system developed by Argonne National Laboratory and deployed widely in the NCSA Alliance. This system will be first installed and evaluated at FSU in first half of year 5. In the following 6 months, we will if the evaluation is positive support installation at other DoD and PET partner sites. Note this is consistent with a slightly less ambitious approach to collaboration than in TangoInteractive. The latter was a fully and elegantly integrated system. Here we use a modular but ad-hoc system of linking together tools from multiple sources without initially an attempt to integrate with a single session management. The latter will be necessary, presumably, for eventual widespread deployment but does not seem to be a requirement for PET and HPCMO use.

9. **Deliverables:**

   - 6 months: Working Access Grid Node at FSU tested and evaluated to other NCSA Alliance Sites
   - 6 months: Evaluation of Access Grid for HPCMO management and training with comparison to desktop systems
   - Contribution to PET Annual Report
   - Written progress report in June 2000
   - Presentation for PET Midyear
   - Final Technical Report

1. **Focused Effort Title:** Collaborative Portals for Training and Computational Science

2. **Organization:** Florida State University

3. **Thematic Area:** HPC Training and DoD User Productivity

4. **PI Names:** Dr. David Bernholdt, Prof. Geoffrey Fox

5. **E-Mail:** bernhold@npac.syr.edu , gcf@cs.fsu.edu

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8. **Statement of Work:**

We are proposing a focused effort supporting two ide as; one is aimed at a prototype "betterportalML" as part of Communication and Collaboration; the second is aimed at a prototype event service as part of Training. Both technologies will be useable in either type of portal.

The new portal architecture has one very important goal - enable users to build new portals very quickly. The result of this focused effort will be both a draft specification of betterportalML but also a prototype "portal construction wizard" that would allow users to choose the objects (and object parameters including layout and collaborative structure) and personal server services and so generate a betterportalML specification of their computing portal. Our idea is that "computer scientists" develop distributed system infrastructure, a nd services. Application scientists define objects (programs, data sets, resources) and can use default or customize portals that use the objects and services. Currently (as in LMS), computer scientists are needed every time one needs a new portal -- in the new approach, application scientists or their staff can build their own portals and define their own objects. New computer science work is only needed when bugs need to be fixed or improved or new services required. Hewlett Packard marketing says that e-Speak is designed to cut construction time of e-commerce sites to 2 hours (a factor of 100 reduction they claim). This focused effort has a similar goal for computing portals. The betterportalML will incorporate the lessons from our year-4 collaborative computing focused effort in terms of XML specification for asynchronous and synchronous collaboration.

Another goal in this focused effort is to build two portal capabilities of relevance to education and training. The result of this will be a system tha t can be used in teaching the same type of material used today but in much more robust environment that supports both asynchronous and synchronous learning. We intend to test the new capability in "collaborative tutorials" offered at ERDC -- initially using tutorials offered by FSU as part of core technology effort. We note that we cannot realistically "quickly replace" systems like TangoInteractive, which have a rich set of capabilities developed over many years. Rather we focus on the most important aspec ts of a Tango session and address these. We think that the two most important aspects of any collaborative training session are the Audio - Video conferencing (discussed separately) and shared curricula (documents). We anticipate

using existing TangoInteract ive or other systems to support shared chat rooms, instant messenger and whiteboards.

The heart of the new portal architecture is a robust queued event system that replaces the server in the TangoInteractive approach. This concept is used to integrate as ynchronous and synchronous collaboration and to support automatic system archiving. We will in first 6 months of this FE develop such a prototype system, which will federate events between the "personal servers" of the new portal architecture. Eventually t his event service will support "all types of objects" (audio -video messages, chat rooms, hand -held prompts, chat -rooms, user customization, server side notification etc.). In this FE, we will aim at two important event capabilities. Firstly the events need ed to support the separate "Hand -Held HPC access FE" and then the harder case of events needed to support both shared pages and tele-pointers for distance learning. This will re -use some of the ideas and perhaps code developed for the "JavaScript Shared Br owser" in TangoInteractive. However rather the fragile JavaScript system implemented in TangoInteractive, we will minimize the browser code and place all the logic on the robust high performance personal server. This will of course make it possible to exp eriment with hand -held devices driven by the same personal server. This will allow the type of collaborative session developed this year as part of "MicroTango FE" but with the new portal architecture.

9. Deliverables:

- 4 months: Prototype definition of be tterportalML
- 6 months: Prototype betterportalML XML to HTML layout tool and Illustrative demonstration of its use in a simple application, Prototype Event Service
- 8 months: Standalone Personal Server Based “JavaScript Shared Browser”, Test of Event Service linking hand -held devices
- 9 months: Prototype betterportalML generation wizard (portal authoring tool)
- 10 months: Test of Event Service linking shared browsers
- 12 months: Use of system in distance learning, Integrated Prototype allowing generation of customizable portal for several applications
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Focused Effort Title:** Ubiquitous Access to HPC Resources
2. **Organization:** Florida State University
3. **Thematic Area:** HPC Training and DoD User Productivity
4. **PI Names:** Dr. David Bernholdt, Prof. Geoffrey Fox
5. **E-Mail:** bernhold@npac.syr.edu , gcf@cs.fsu.edu
6. **Telephone:** (315) 443-3857, (850) 644-4587
7. **Fax:** (315) 443-1943, (850) 644-0098
8. **Statement of Work:**

Given the work going on in the "computing portals" world (activities supported by DoD, DOE, NSF, industry, etc.), it makes sense to envision the connectivity to HPC resources as services offered by a portal, and the handheld simply as a device with a particular set of capabilities that can link with the portal server. In this way the services don't have to be implemented separately for every different display device that comes along, and the portal can act as a flexible gateway to accommodate the different capabilities of various display devices.

This project will demonstrate connectivity between HPC job and status information and handheld devices. In keeping with the portal/gateway concept described above, traditional web browser based access to the same information will be provided, but it will not be the primary focus of this project. Information available will include job initiation, progress, and termination (such as can be obtained from the batch queuing system). We will also investigate the possibility of including user-provided data, for example, periodically providing the trailing few lines of the job's output file. Two-way interaction, such as user job cancellation and simple steering, will also be considered in the design, but will not be implemented unless we find a way to do this in general, taking into account security considerations.

The emphasis of this work will be on the architecture and design of the gateway which links the handheld device to the fixed information base. To accommodate the intermittent nature of communications with most handheld devices, the gateway will have to queue messages for delivery, and will have the ability to filter/transform messages based considerations of both the display device and "quality of service", for example, for messages which periodically monitor the progress of a job, usually all but the most recent can be dropped, while other messages should be transmitted regardless. The gateway will be designed to accommodate a broad range of handheld devices and communications channels ranging from pagers (gateway pushes messages to device, but functionality is extremely limited) to personal digital assistants (gateway generally waits to be polled, but much more functionality is possible). We will emphasize the use of commodity/standard tools and technologies; the emerging Wireless Application Protocol (WAP) is of particular importance at this stage since it appears to have substantial momentum and significant functionality.

9. Deliverables:

- Demonstration of HPC job information gateway for hand -held devices
- Assistance with installation of the system at ERDC MSRC, if desired
- Contribution to PET Annual Report
- Written progress reports in June and December 20 00
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report assessing security and hand -held devices in the DoD HPCMP context, March 2001

1. **Focused Effort Title**: Computational Science and Information Te chnology: Curriculum and Technology

2. **Organization**: Florida State University

3. **Thematic Area**: HPC Training and DoD User Productivity

4. **PI Name**: Prof. Geoffrey Fox

5. **E-Mail:** gcf@cs.fsu.edu

6. **Telephone**: (850) 644-4587

7. **Fax**: (850) 644-0098

8. **Statement of Work**:

We describe a new curriculum (Computational Science and Information Technology) being developed at Florida State University. The curriculum consists of four courses:

1) Computational Science I
2) Computational Science II
3) Applied Information Technology I
4) Applied Information Technology II

We argue that it could be of particular value to HBCU/MI's and to DoD scientists and engineers. This value will be enhanced if the curriculum is made available by distance education technology . In this project, we take this basic thesis and we investigate its value to the ERDC Graduate Institute. We do this in a way that will test technology that is being developed in other focused efforts. This semester we taught a class to several sites including JSU and the ERDC Graduate Institute. We used TangoInteractive technology and although adequate, the class was disappointing in its lack of interactions between students and teacher. When the class was given at ERDC there were many interactions with students. When giving the class from Syracuse or Tallahassee, there were essentially no questions from any remote site. We have proposed in other focused efforts, a different strategy from Tango, which involves a mix of synchronous and asynchronous interacti ons with lectures available in SMIL format for students to peruse before tutorial sessions held synchronously. We have also proposed developing novel applications of hand -held devices.

9. **Deliverables:**

- September 2000: Technology Framework and Curriculum D esign
- December 2000: Graduate class developed and adapted for ERDC Graduate Institute
- January-April 2001: Delivery of prototype class at ERDC Graduate Institute
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Focused Effort Title:** Standard File Format for Large Data Problems and Visualization

2. **Organization:** NCSA, University of Illinois at Urbana-Champaign

3. **Thematic Areas:** Management and Interpretations of Large Data Sets, SciVis for Very Large Problems

4. **PI Names:** Dr. Polly Baker, Dr. Mike Folk

5. **Email:** baker@ncsa.uiuc.edu, mfolk@ncsa.uiuc.edu

6. **Telephone:** (217) 244-1997, (217) 244-0647

7. **Fax:** (217) 244-2909, (217) 244-1987

8. **Statement of Work:**

This initiative is a collaboration between NCSA and the ERDC Coastal and Hydraulics Lab to investigate the use of NCSA's HDF5 file format to address the need for efficient access and storage of data generated and used by CH3D surface water modeling code.

The CH3D-SED numerical modeling system is being utilized to investigate sedimentation on bendways, crossings, and distributaries on the lower Mississippi and Atchafalaya Rivers. This involves very large, multi-layered time-sequenced datasets. These datasets also often contain many sparse regions. Current formats and access software for the system are raw Fortran data files and do not support data compression. As a result data storage requirements are high, and data processing can be very slow, and partial data access, such as extractions of small subsets of the data, can take a great deal of time. The format also does not lend itself to the I/O demands of parallel computing environments.

The HDF5 data format and I/O library is designed to address precisely these problems. HDF5 can store datasets of virtually any size, supports sparse data storage efficiently, provides structures that facilitate efficient partial access, as well as parallel I/O.

In this project, NCSA will work with investigator Ronald Heath of the ERDC Coastal and Hydraulics Lab. We will identify storage structures in HDF5 that will support efficient storage and access to CH3D data. Using these storage structures, we will test the efficiency and usability of the HDF5 format for typical CH3D application. If this work indicates that HDF5 can indeed result in significant improvements, we will identify alterations that need to be made to both HDF5 and CH3D to produce an HDF5 interface to CH3D.

9. **Deliverables:**

- Report design of experimental HDF5 file structures for CH3D (July 2000)
- Report on results of testing and recommendations regarding further integration of CH3D and HDF5 (October 2000)
- Contribution to PET Annual Report
- Written progress reports in June and December 2000

- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

ERDC MSRC PET YEAR FIVE EFFORTS

1. **Core Support Area:** HPC Support for HBCU/MIs

2. **Organization:** Jackson State University

3. **Lead:** Prof. Willie G. Brown

4. **E-Mail:** wbrown@jsums.edu

5. **Telephone:** (601) 979-4300

6. **Fax:** (601) 979-4301

7. **Statement of Work:**

   Jackson State University (JSU) will continue to provide a core level of effort to support student training activities at JSU. This will include HBCU/MI web page maintenance and updating, HBCU/MI capabilities database, users group meetings, visits to ERDC MSRC and conduct of the Summer Institute, including student recruitment, student room, board, and stipends, presenter/instructor scheduling and coordination, and course materials and supplies.

8. **Deliverables:**

   - HBCU/MI Web Pages
   - HPC Summer Institute
   - Reports on HBCU/MI Activities
   - Attendance and participation in PET meetings, conferences, workshops, colloquia, etc.
   - Contribution to PET Annual Report
   - Written progress reports in June and Decembe r 2000
   - Presentations for PET Midyear and Annual Reviews

ERDC MSRC PET YEAR FIVE EFFORTS

1. **Core Support Area:** PET Academic Lead
2. **Organization:** ERC, Mississippi State University
3. **Lead:** Prof. Joe Thompson
4. **E-Mail:** joe@erc.msstate.edu
5. **Telephone:** (601) 325-7299
6. **Fax:** (601) 325-7692
7. **Statement of Work:**

   MSU ERC will continue to provide a core level of effort to support the academic leadership of the PET program at ERDC MSRC. Responsibilities include, but are not limited to, participation in the Academic Executive Committee (ExComm) for PET across the four MSRC's; maintaining knowledge of current status of all Focused Efforts ongoing at the (currently) eleven participating university partners; review and recommendations for funding of PET Focused Efforts and participation in planning and execution of PET meetings (Midyear Review, Annual Review, workshops, DoD Users Meeting, etc.), as appropriate. MSU ERC will select and attend conferences and other meetings that have high payoff and direct application for the PET Program.

8. **Deliverables:**

   - Trip reports for conferences and user contacts (as conducted)
   - Annual Report
   - Written progress reports in June and December 2000

ERDC MSRC PET YEAR FIVE EFFORTS

1. **Core Support Area:** Computational Fluid Dynamics (CFD)
2. **Organization:** ERC, Mississippi State University
3. **Lead:** Prof. Bharat Soni
4. **E-Mail:** bsoni@erc.msstate.edu
5. **Telephone:** (601) 325-2647
6. **Fax:** (601) 325-7692
7. **Statement of Work:**

   MSU ERC will continue to provide a core level of effort to support the CFD on -site position for the PET program at ERDC MSRC. MSU will provide a core level of effort to support technology transfer, user outreach, training and assessment of targeted codes and algorithms in CFD. Targeted codes include, but are not limited to the CFD CHSSI co des. Technology of interest includes, but is not limited to, grid generation codes, parallelization of CFD algorithms, numerical solvers, management and interpretation of large data sets, adaptive and meshless techniques, etc. MSU will maintain frequent contact with the DoD CTA Lead for CFD. MSU will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer.

8. **Deliverables:**

   - Trip reports for conferences and user contac ts (as conducted)
   - Contributions to PET website for CFD as appropriate
   - CFD Training Course
   - Support for JSU HPC Summer Institute
   - Contribution to PET Annual Report
   - Written progress reports in June and December 2000
   - Presentations for PET Midyear and Annual Rev iews
   - At least one technical report by on -site lead

ERDC MSRC PET YEAR FIVE EFFORTS

1. **Core Support Area:** Computational Structural Mechanics (CSM)
2. **Organization:** ERC, Mississippi State University
3. **Lead:** Prof. Joe Thompson
4. **E-Mail:** joe@erc.msstate.edu
5. **Telephone:** (601) 325-7299
6. **Fax:** (601) 325-7692
7. **Statement of Work:**

   MSU ERC will continue to provide a core level of effort to support the CSM on -site position for the PET program at ERDC MSRC. MSU will provide a core level of effort to support technology transfer, user outreach, training and assessment of targeted codes and algorithms in CSM. Targeted codes include, but are not limited to, EPIC, CTH, DYNA3D, and NASTRAN. Technology of interest includes, but is not limited to, grid generation codes, management and interpretation of large (terascale) data sets, adaptive and meshless techniques, etc. MSU will maintain frequent contact with the DoD CTA Lead for CSM to understand the priorities and ongoing CHSSI activities. MSU will select and attend focused conferences and other meetings th at have high payoff and direct application for user interaction and technology transfer.

8. **Deliverables:**

   - Trip reports for conferences and user contacts (as conducted)
   - Contributions to PET website for CSM as appropriate
   - Contribution to PET Annual Report
   - Written progress reports in June and December 2000
   - Presentations for PET Midyear and Annual Reviews
   - At least one technical report by on -site lead

1. **Focused Effort Title:** Grid Assembly Enhancements for Chimera Technology

2. **Organization:** ERC, Mississippi State University

3. **Thematic Areas:** HPC Training and DoD User Productivity, HPC Performance Metrics/Tools

4. **PI Name:** Prof. Bharat Soni

5. **E-Mail:** bsoni@erc.msstate.edu

6. **Telephone:** (662) 325-2647

7. **Fax:** (662) 325-7692

8. **Statement of Work:**

Under the current effort, the grid assembly process will be studied, analyzed and improved for both node centered and cell centered flow solvers with focus on large scale applications. In particular, we will concentrate on the data structures and algorithms used for grid assembly including polygonal mapping (PM) trees, Cartesian inverse maps, hole cutting, and stencil searching, etc.

We propose to develop techniques to visualize the appropriate data structures in order to improve the processes of debugging grid assembly problems and developing grid assembly algorithms. We will analyze the effects of round-off errors encountered during the construction of the appropriate data structures.

We will analyze the strengths and weaknesses of the hole cutting algorithms used in different grid assembly codes including the opportunities offered for parallel execution. Results from the CTK development project will be leveraged in this development and vice versa. The enhancements and improvements made in this development will be validated using the BEGGAR and OVERFLOW-D codes. We will work very closely with Robert Meakin (U.S. Army) for his expertise in the development of OVERFLOW-D, Jubraj Sahu (ARL) who directs a challenge project on the full trajectory simulation of a missile with actively controlled fins, Ralph Noack (Eglin AFB) for his expertise in the development of BEGGAR, Michael Aftosmis (NASA Ames) for his expertise in round-off errors encountered in clipping faceted geometry and Robert Nichols (AEDC) for his expertise in Chimera based flow solvers and PEGSUS.

9. **Deliverables:**

- A software module for the visualization of a polygonal mapping tree and the interactive classification of points using this data structure
- Validation and demonstration of the enhancements in grid assembly for addressing large scale applications using BEGGAR and OVERFLOW-D
- A conference paper and ERDC report with documentation of the polygonal mapping tree visualization software
- Contribution to PET Annual Report

- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report with an in-depth survey of hole cutting algorithms and their role in grid assembly for Chimera technology

1. **Focused Effort Title:** Java Based CFD Training
2. **Organization:** ERC, Mississippi State University
3. **Thematic Area:** HPC Training and DoD User Productivity
4. **PI Name:** Prof. Bharat Soni
5. **E-Mail:** bsoni@erc.msstate.edu
6. **Telephone:** (662) 325-2647
7. **Fax:** (662) 325-7692
8. **Statement of Work:**

   We propose to develop a WEB based CFD training and demonstration tool for students and non-CFD users. This tool will utilize a JAVA based graphical user interface and will provide interactive visualization and control various paramete rs (boundary conditions, geometry, grid, flow variables to visualize, numerical scheme to exercise, dissipation order to apply, angle of attack, contour vs. line plots, etc.). The software will contain various numerical schemes, boundary conditions and mac ros for geometry and grid information. The MIT tool, jvwt, will be used as a basis. However, this tool will be enhanced to provide links with the MSU hybrid grid and flow solver and the WEB based grid training tool being developed in conjunction with the W EB based grid generation code. The students will be able to exercise "what if" scenarios with respect to grid, BCs and flow parameters.

9. **Deliverables:**

   - A WEB based CFD demonstration and training tool with interactive setup of grid, BCs and flow parameters and visualization of the CFD process
   - On-line documentation and help
   - A training tool demonstration at JSU, CAU and Morgan State University
   - Contribution to PET Annual Report
   - Written progress reports in June and December 2000
   - Presentations for PET Midyear an d Annual Reviews
   - Final Technical Report with the description of the training tool

1. **Focused Effort Title:** Library of Interpolation and Approximation Modules (INLiB **)**
2. **Organization:** ERC, Mississippi State University
3. **Thematic Area:** HPC Training and DoD User Productivity
4. **PI Name:** Prof. Bharat Soni
5. **E-Mail:** bsoni@erc.msstate.edu
6. **Telephone:** (662) 325-2647
7. **Fax:** (662) 325-7692
8. **Statement of Work:**

The development of INLiB (Interpolation and approximation library) is a proposed collaborative effort of the ERC, Mississippi State University, and TICAM, University of Texas at Austin. This library will contain stand-alone interpolation and approximation modules providing various functionalities associated with numerical simulations for CFD, CSM, EQM and other CTAs. The library modules will be accessible from FORTRAN, C and C++ applications via APIs. For example, the modules will contain:

1) Linear, bilinear, trilinear, Bezier, B-spline and NURBS interpolation and approximation functions
2) Interpolation/approximation of various geometric entities into NURBS representation
3) Interpolation modules used for generation of structured grids(transfinite interpolation, transformations, …)
4) Interpolation of solution properties between distinct grid strategies/resolutions
5) Feature detection module
6) Weighted interpolation/approximation of solution characteristics addressing conservative properties

9. **Deliverables:**

- A software package containing INLiB and associated documentation
- Validation and demonstration of INLiB for DoD applications
- A conference paper summarizing INLiB development
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report with in-depth description of interpolation/approximation algorithms

1. **Core Support Area:** Climate/Weather/Ocean Modeling and Simulation (CWO)
2. **Organization:** Ohio State University
3. **Leads:** Prof. Keith W. Bedford, Prof. Ponnuswamy Sadayappan
4. **E-Mail:** bedford.1@osu.edu; sadayappan.1@osu.edu
5. **Telephone:** (614) 292-7338, (614) 292-0053
6. **Fax:** (614) 292-3780
7. **Statement of Work:**

   OSU will continue to provide a core level of effort to support technology transfer, user outreach, training, and assessment of targeted codes and algorithms in CWO. Targeted codes include, but are not limited to, WAM, CH3D, SWAN, SED, FRM, MMS, and COSED. Technologies of interest include, but are not limited to, application of circulation and wave models to sea condition prediction; coupling of wave, sediment and circulation models; etc. OSU will maintain frequent contact with the DoD CTA Lead for CWO to understand the priorities and ongoing CHSSI activities, as well as with the local CWO representative at ERDC MSRC. User outreach will also consist of presentations at the DoD HPC Users Group Conference and a series of PET CWO training courses. OSU will select and attend focused conferences and other meetings that have high payoff and direct application for use interaction and technology transfer.

8. **Deliverables:**

   - Produce multithreaded version of SC-MICOM
   - Monthly updates of CWO material on ERDC PET web site
   - CWO training courses
   - Presentation at DoD HPC Users Group Conference
   - Contribution to PET Annual Report
   - Written progress reports in June and December 2000
   - Presentations for PET Midyear and Annual Reviews
   - At least one technical report by on-site lead

1. **Focused Effort Title:** Enhancement, Evaluation, and Application of a Coupled Wave Current-Sediment Model for Nearshore and Tributary Plume Predictions

2. **Organization:** Ohio State University

3. **Thematic Areas:** HPC Training and DoD User Productivity, Scalable Computing Migration

4. **PI Names:** Prof. Keith W. Bedford, Prof. Ponnuswamy Sadayappan

5. **E-Mail:** bedford.1@osu.edu, sadayappan.1@osu .edu

6. **Telephone:** (614) 292-7338, (614) 292-0053

7. **Fax:** (614) 292-3780

8. **Statement of Work:**

The accurate prediction of sediment transport and suspended sediment concentrations are important issues for a number of military activities. These activ ities include navigation channel maintenance and dredged material disposal, and the prediction of submarine sediment clouds in which vessels and/or submerged assault troops can elude detection. Both wave and current motions cause sediment transport and sus pension, but in traditional models only current-induced effects have been considered. In coastal waters, wave effects become important and their inclusion can greatly improve the accuracy of sediment predictions.

In PET year 4, the ERDC MSRC program suppo rted the development of a parallel-processing, coupled wave-current bottom boundary layer modeling system. This system involves the WAM wind-wave model, the CH3D-SED circulation and sediment transport model, and the WCBL wave-current boundary layer model. WCBL receives input fields of wave, current, and sediment properties from the WAM and CH3D -SED models. It then simulates a nonlinear, coupled bottom boundary layer, including sediment -induced stratification, and returns improved estimates of bottom shear s tress and bottom roughness to CH3D-SED and bottom friction factor to WAM.

The coupled WAM/CH3D-SED/WCBL system was deployed for the Adriatic Sea in PET year 4. The results of a hindcast for one week in February 1999 indicated that application of the combined boundary layer model resulted in increases in CH3D -SED suspended sediment concentrations of more than 200% in shallow water under the influence of large waves. Unfortunately no sediment data is available at that site for verification and this poses two difficulties in evaluating model performance. First, to date the impact of the coupling appears to be excessive. This is suggested by large spatial gradients in sediment concentration and lack of WCBL convergence when wave-induced bottom velocities domina te bottom currents. Second, the mobile bed portion of the CH3D -SED model has never been tested. Such tests are critical as representation of the bedforms, sorting, and roughness is crucial to the success of the coupled model. Therefore, additional research is required to refine and verify the WCBL and mobile bed models.

This Focused Effort proposes to continue WCBL development by improving algorithm accuracy and verifying predictions using wave, current, and sediment data from the Dredging Operation and Environmental Research (DOER) experiment, funded by the U.S. Army Corps of Engineers (USACE). The DOER experiment will be performed in the 2000 field season and will involve the evaluation of nearfield dredged material placement at the ERDC Field Research Facility (FRF) at Duck, NC. The aim of this experiment is to refine ERDC scientists' ability to predict the behavior of dredged material placed offshore, with a view to better planning and management of dredging operations. Dr Jack Davis (ERDC) is coordinating dredged material placement and data collection efforts at the FRF. Dr. Joe Gailani (ERDC) is performing the local disposal site modeling aspect of the experiment using the USACE Long Term Fate (LTFATE) sediment transport model. He also sees great benefit in having simulations made using the WAM/CH3D-SED/WCBL system, which contains more advanced physics and covers a larger domain than LTFATE. Validation of the WAM/CH3D-SED/WCBL system would provide the USACE with an advanced tool for predicting dredged material transport. Dr. William Birkemeier manages the ERDC FRF and he has also expressed support for the use of the coupled system in connection with the DOER experiment
.

The SED sediment-modeling component of CH3D-SED simulates erosion, deposition, and transport processes for multiple sediment size classes. It does not, however, model the consolidation, and associated settling, of bed sediment. This process is important in dredged material disposal and river plume situations. Measurements taken within the DOER experiment's dredged material disposal mound will permit calculation of the consolidation of the sediment material and its incorporation into the coupled model through a Been and Sills mechanistic formulation. The use of this mechanistic description is the first such in any large-scale water body model.

In PET year 4, Dr. Peter Orlin of the Ocean Products Division (OPD) at NAVOCEANO approached the OSU WCBL development team. Dr. Orlin is interested in using the WAM/CH3D-SED/WCBL system to model coastal and riverine sediment plumes thereby enhancing the ability of the OPD to predict marine circulation and acoustic response for various U.S. Navy projects. This Focused Effort will provide support to Dr. Orlin in this endeavor.

9. Deliverables:

- Deployment of WAM, CH3D-SED, and WCBL models on appropriate grids for FRF experiment (5/2000)
- Refinement of WCBL algorithm for high waves/low current case (7/2000)
- Addition of consolidation model to CH3D-SED model (9/2000)
- Preparation of input files based on FRF experiment data (9/2000)
- Hindcast of FRF experiment (11/2000)
- Analysis of FRF experiment hindcast (1/2001)
- Tuning of WCBL based on FRF experiment hindcast (3/2001)
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Focused Effort Title:** HPC Training Courses
2. **Organization:** Ohio Supercomputer Center
3. **Thematic Area:** HPC Training and DoD User Productivity
4. **PI Names:** Dr. Richard Pritchard, Ms. Leslie Southern
5. **E-Mail:** rhp@osc.edu, leslie@osc.edu
6. **Telephone:** (614) 292-9248, (614) 292-9248
7. **Fax:** (614) 292-6870
8. **Statement of Work:**

Provide quality training by experienced instructors for the DoD HPC Community. OSC has provided heterogeneous high-performance computing facilities and services to a statewide community for over 10 years and more recently a broader national community through the DoD Modernization Program and the National Computational Science Alliance. Training offerings are developed and designed specifically for the HPC user community. Instructors are both experienced HPC specialists and experienced users and are not economically bound to any one vendor or vendor product.

Contract Year 5 OSC Training Courses:

Using the Cray T3E for Code Development and Analysis
Length: 2 days
Approximate Date: Any time
Description: This course covers a range of hardware and software features available to users of the Cray T3E. The topics covered include hardware, operating system, interactive usage, process management, environment management, batch processing, compilers, debugging tools, performance analysis tools, timing routines, single-node numerical libraries, parallel numerical libraries, fine-grained parallelism, data locality, and streams.

Using the SGI Origin 2000 for Code Development and Analysis
Length: 2 days
Approximate Date: Any time
Description: This "hands-on" course covers an extensive range of hardware and software features available to users of the SGI Origin 2000(O2K). The topics covered are: introduction to the O2K; the MIPS R10000 Processor; the architecture of the O2K; an introduction to the IRIX operating system; programming environment; compiling systems (including "useful" options); batch processing; single-processor performance analysis tools; SGI data distribution directives; automatic parallelization; message passing libraries for parallel programming; debugging tools.

The format of the course will consist of lectures on these topics as well as lab sessions in which participants will write their own parallel code and run software tools.

Multilevel Parallel Programming
Length: 2 days
Approximate Date: After June 2000
Description: This course is intended as an introduction to multilevel parallel progr amming, a style of parallel programming in which both message passing techniques (such as MPI) and shared memory techniques (such as OpenMP or Pthreads) are used. This allows high performance codes to best take advantage of the distributed/shared memory a rchitectures of modern parallel supercomputers such as SGI Origins, IBM Power3 SMPs, and clusters of commodity SMP systems. Users will learn how to apply multilevel parallel programming techniques to their problems of interest, how to optimize these techn iques for different architectures, and how to avoid potential problems. Topics covered include: introduction to distributed/shared memory architectures; overview of message passing techniques; overview of shared memory techniques; mixing message passing an d shared memory; optimization techniques; examples.

C++ for Scientists
Length: 3 days
Approximate Date: July 2000
(Note: This course is being offered at the ASC MSRC. OSC instructors are experienced with distance learning technologies, such as Tango Inte ractive 2.0 (TI 2.0). With the permission and assistance from ASC MSRC staff, OSC will provide this course via TI 2.0 to the ERDC MSRC.)
Description: This course teaches the philosophy and syntax of the C++ programming languages. Special emphasis will be p laced on two areas: improvements to the C programming language found in C++, and the object -oriented programming features of C++

Since the object-oriented approach to writing code is a new technique for many users, the course offers a description of and rationale for this powerful programming style. In terms of the C++ language in particular, the following topics will be covered: the class data type for object creation and use, the various types of C ++ functions, function and operator overloading, inheri tance and class hierarchies, the C++ I/O stream, and abstract data types.

9. Deliverables:

Course announcements and electronic copies of training materials for each course prior to each course date. All courses are available in Microsoft PowerPoint and a combination of HTML and JPEG files. The web pages are designed to move sequentially through course materials and contain embedded links in table of contents and section indices. This provides the student the flexibility to jump to particular sections o f interest.

ERDC MSRC PET YEAR FIVE EFFORTS

1. **Core Support Area:** Scalable Parallel Programming Tools
2. **Organization:** Rice University
3. **Lead:** Dr. Richard Hanson
4. **E-Mail:** koolhans@cs.rice.edu
5. **Telephone:** (713) 285-5868, (713) 285-5304
6. **Fax:** (713) 285-5136
7. **Statement of Work:**

Rice will continue to provide support in the general areas of technology transfer, user and community outreach, and training in new technologies related to SPP tools. The tools include parallel debugging tools, parallel application development software librarie s, and access to expertise in key areas of importance to ERDC MSRC and its DoD clients. Rice will coordinate tools activities by the PET team at Rice and University of Tennessee, and provide on-site tools support through Dr. Clay Breshears. At -Rice researchers will work with Clay to engage users, provide technology transfer, and focus on MSRC needs. Rice personnel will attend related meetings and conferences that support the ERDC MSRC user mission. For each such trip Rice will submit, in advance, a ration ale to allow NRC management to determine the coverage of ERDC MSRC PET funds for the related expenses.

Work begun on assisting ERDC CHL researchers to achieve high performance on the STWAVE code will continue. Such efforts will be carried out in associ ation with the efforts of PET CWO personnel involved with improvements to the physics of the code. Migration of the SCMICOM code to use Pthreads will also be undertaken in conjunction with the on -site PET CWO Lead. Work on other codes, identified by ERDC M SRC management as having high priority, will also be carried out as possible.

A movement of application codes (such as DoD Challenge projects) to the just installed IBM POWER3 architecture is expected to occur during this year. In order to make the most effective use of this new computing platform, codes may need redesigned algorithms for the distributed-shared memory architecture. The nature of such work would involve analysis of function evaluations, use of parallel programming tools, including the use of Pthreads and OpenMP, and message passing as appropriate for achieving high performance. On-site and at-Rice personnel have the necessary expertise in these areas and will be available to assist users in their code migration.

Training for this year will involve courses on programming tools that are available on ERDC MSRC HPC platforms. The potential topics include such things as performance analysis tools (e.g., VAMPIR, SGI SpeedShop), debuggers (e.g., TotalView), and concurrent programming models (e.g., Pthreads, OpenMP). Other related tools and topics, such as software libraries, may be offered dependent upon amount of interest from ERDC MSRC users.

8. Deliverables:

- Trip reports for conferences and user contacts
- Training Courses
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- At least one technical report by on-site lead

1. **Focused Effort Title:** Parallel IO

2. **Organization:** University of Tennessee, Knox ville

3. **Thematic Areas:** HPC Training and DoD User Productivity, Management and Interpretation of Large Data Sets

4. **PI Name:** Dr. Graham E. Fagg

5. **E-Mail:** fagg@cs.utk.edu

6. **Telephone:** (865) 974-5790

7. **Fax:** (865) 974-8296

8. **Statement of Work:**

This project will aim to accomplish three main objectives:

1) To evaluate and performance test the vendor parallel IO subsystems installed on the EDRC MSRC platforms, as they would be utilized by current system users (i.e., high -level API access from MPI 2 for example).
2) To educate users on the benefits of using such parallel IO systems.
3) To demonstrate benefits to users by tuning an existing DOD Challenge application that is currently "IO bound" and by assisting with use of MPI 2 parallel IO in th e EQM CE-QUAL-ICM code.

Justification, benefits and comments:

1) Validation of the vendor installed IO sub -systems will build confidence in the current user community and system support staff that the IO subsystems are installed correctly and that when used correctly they can potentially offer sizeable performance benefits for many application classes.
2) Educating users is required as many users have never had real exposure to a truly parallel file system at the library API level before, especially in the case of users of the more traditional vector systems. Even experienced scalable system users need to be warned of potential pitfalls and expected realistic performance gains versus the development effort required.
3) Validation of required effort versus performa nce for actual user applications will not only benefit users directly, as well as allow for better system throughput of applications on the EDRC MSRC systems, but will also act as a more thorough test of the system than can either a benchmark or validation suite.

9. **Deliverables:**

- Benchmark results for parallel IO subsystems
- Training course on parallel IO
- Collaboration with EQM code developers on use of MPI -2 parallel IO
- Contribution to PET Annual Report

- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Focused Effort Title**: Metacomputing Support for the SARA-3D Structural Technology Acoustics Application

2. **Organization**: University of Tennessee, Knoxville

3. **Thematic Areas**: Scalable Computing Migration, Management and Interpretation of Large Data Sets

4. **PI Name:** Dr. Shirley V. Browne

5. **E-Mail:** browne@cs.utk.edu

6. **Telephone:** (865) 974-3547

7. **Fax**: (865) 974-8296

8. **Statement of Work**:

This project will use the NetSolve MATLAB interface to provide access to MSRC HPC platforms for users of the SARA-3D structural acoustics code. NetSolve is a client/server system that provides access to HPC hardware and software from familiar desktop environments, using a variety of client interfaces, including Fortran, C, and Java programming interfaces, and MATLAB and Mathematica interactive interfaces. Initially NetSolve will be used to allow the computationally intensive portions of the MATLAB-based post-processing for SARA-3D to be carried out on ERDC HPC machines, while allowing users to run their MATLAB programs as usual from their desktop machines. Invocation of the computationally intensive routines will be implemented by remote procedure calls to versions of these routines installed on a NetSolve server. This approach will allow interactive use of HPC resources to improve real-time response for the post-processing and visualization of large-scale SARA-3D output data.

SARA-3D outputs a very large file that provides surface pressures and surface velocities at the fluid-structure interface as a function of frequency. This file may then be used to calculate the following quantities:

1. Fully three-dimensional representation of field pressures in the nearfield as a function of frequency,
2. Fully three-dimensional representation of field pressures in the farfield as a function of frequency,
3. Fully three-dimensional representation of radiated power as a function of frequency.

Currently, the SARA-3D post-processing is done on large HPC machines using non-parallel FORTRAN-based subroutines which output a MATLAB data file that is then transferred back to the user's home machine. This method of getting field pressures and radiated power works, but is inefficient. The idea using NetSolve would be as follows: when the need arises for a user to perform post-processing (1, 2, or 3 above), he would open a MATLAB application on his home machine and access the dataset at ERDC MSRC via NetSolve. Since each calculation of field pressure (i.e., each point in both space and time) is totally independent of the other calculation, we expect that the NetSolve task farming

capability could be used to achieve parallelism, which should dramatically improve post-processing response time.

UTK and BBN Technologies propose to collaborate on the following three-phase approach to improving the scalability and usability of SARA-3D. First, a NetSolve post-processing routines for 1, 2, and 3 above will be implemented on the NetSolve server, using the NetSolve task farming interface to achieve parallelism. Second, SARA-3D users will be trained in the use of the NetSolve MATLAB interface for post-processing SARA-3D output. Third, the NetSolve MATLAB interface will be applied to other DoD projects using MATLAB.

9. Deliverables:

- NetSolve server implementation of SARA-3D post-processing routines
- Demonstration of use of the NetSolve MATLAB interface to invoke SARA-3D post-processing
- NetSolve tutorial at either ERDC or a location convenient to SARA-3D users
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

ERDC MSRC PET YEAR FIVE EFFORTS

1. **Core Support Area:** Computational Structural Mechanics (CSM)
2. **Organization:** TICAM, University of Texas at Austin
3. **Lead:** Prof. Tinsley Oden
4. **E-Mail:** oden@ticam.utexas.edu
5. **Telephone:** (512) 471-3312
6. **Fax:** (512) 471-8694
7. **Statement of Work:**

TICAM will continue to provide a core level of effort to support technology transfer, user outreach, and training. Technology of interest includes, but is not limited to, adaptive mesh and grid algorithms and tools, management of large CSM data sets, and parallelization/coupling of key CSM codes. Texas will maintain regular contact with Dr. Richard Weed, the ERDC MSRC PET On-site Lead for CSM, to facilitate technology transfer, user outreach, and relevance to current MSRC issues. Related codes include CTH, EPIC and DYNA3D. During the year, TICAM will make site visits to ERDC MSRC to work with the DoD users and on-site personnel for CSM.

TICAM will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. For each conference attended, Texas will submit in advance a "statement of benefits" to PET that allows the NRC management to determine whether ERDC MSRC PET funding should be used to cover the cost of that meeting. Targeted training includes, but is not limited to, training courses/workshops on grid generation, adaptive grids, management of large data sets, and efficient reliable HPC computations. Such training may be conducted either at ERDC MSRC or at remote user sites as deemed necessary and appropriate. TICAM will work with the On-site Academic Lead to arrange training classes during the year.

8. **Deliverables:**

- One or more papers or poster sessions will be submitted for presentation at next DoD HPC Users Group Conference
- One or more papers will be submitted for presentation at Supercomputing 2000
- Trip reports for conferences and user contacts (as conducted)
- Contributions to CSM portion of ERDC PET website
- One or more papers will be presented at HPC2000
- Special sessions on CSM hydrocode simulation and on unstructured grids and parallel partitioning will be organized for FEF2000 (to be held in Austin, TX, April 1-4, 2000)
- Workshop may be conducted on adaptive grids, modeling and algorithms for CSM
- Shortcourse or shortcourses will be held at Vicksburg on CSM hydrocode simulators and methodology and on parallel frameworks and software
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews

1. **Focused Effort Title:** AMR and CTH Capability and Algorithm Enhancements
2. **Organization:** TICAM, University of Texas at Austin
3. **Thematic Area:** Scalable Computing Migration
4. **PI Names:** Prof. Graham Carey, Prof. Tinsley Oden
5. **E-Mail:** carey@cfdlab.ae.utexas.edu, oden@ticam.utexas.edu
6. **Telephone:** (512) 471-4676, (512) 471-3312
7. **Fax:** (512) 232-3357, (512) 471-8694
8. **Statement of Work:**

   The focus of this part of the work is enhancement of the capabilities of DoD codes such as CTH to meet some of the needs expressed by DoD users at the recent PET Annual review. We have been expanding the CTH software framework to include adaptive mesh refinement (AMR). We are also working with software developers at Sandia on parallel aspects of the study. The present component of the work deals with problems related to application programming interfaces to support: (1) improved capabilities to handle rigid obstacles of arbitrary shape in CTH; and (2) improved extraction of pressure-field data for interfacing with other DoD application codes (for example, DYNA). A second part of the work concerns the development of improved algorithms and, particularly, improved time integration procedures. This is a major stumbling block to efficient simulation: as the cells deform in Lagrangian calculations or are repeatedly refined in the Eulerian simulations the timestep is adversely affected. We plan to study this problem and develop strategies for resolving or ameliorating it. This work will be conducted in the latter part of the year and depending on the outcome could become a major focused effort in the following year. The testbed will be utilized for some of these studies to expedite development and testing of ideas.

9. **Deliverables:**

   - Contributions to PET CSM web page on capability enhancements, algorithms, test problems, and performance results
   - Conference papers and journal articles detailing results of the project, expanded capabilities, new algorithm development, analysis, performance and application studies
   - Software for enhancements with supporting technical documentation in testbed
   - Visit to Vicksburg and briefing to ERDC MSRC on research progress
   - Contribution to PET Annual Report
   - Written progress reports in June and December 2000
   - Presentations for PET Midyear and Annual Reviews
   - Final Technical Report

1. **Focused Effort Title:** Adaptive Mesh Technology, Mesh Improvement and Algorithms for Hypervelocity Impact and Penetration Analyses

2. **Organization:** TICAM, University of Texas at Austin

3. **Thematic Area:** Scalable Computing Migration

4. **PI Names:** Prof. Graham Carey, Prof. Tinsley Oden

5. **E-Mail:** carey@cfdlab.ae.utexas.edu, oden@ticam.utexas.edu

6. **Telephone:** (512) 471-4676, (512) 471-3312

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8. **Statement of Work:**

TICAM will expand on and extend our recent work to promote and develop unstructured grid approaches and adaptive mesh refinement methods for CSM codes used by DoD researchers in hypervelocity impact and penetration analyses. Both Eulerian and Lagrangian approaches and their derivatives (ALE codes) are impacted by this research effort. In support of this need, TICAM has been developing local mesh refinement strategies for these analysis codes and investigating data structure issues related to implementation of various refinement strategies. The DoD codes CTH and EPIC are the primary test codes for this work. The work will be further developed and refined under the proposed project and will also focus on several issues of immediate interest to the gridding and finite element analysis needs of the Structures Lab users at ERDC. Additional work on local error indicators of residual types will be formulated and analyzed and we will continue the work on recovery-type indicators with emphasis on implementation and testing within the frameworks of the designated test codes. The work on the Lagrangian analysis codes involves deforming grids and an assessment of shape quality of the elements as the solution and grid evolve. The framework of the Eulerian computational testbed which was commenced in last years funding will be completed early in the funding year and tests with error indicators for "basic physics" including shock layers will be carried out. The performance of different indicators and comparison tests with known analytic solutions will be conducted to validate code and verify/test the indicators. This will then be utilized to enable rapid evaluation of indicators and algorithms for very large codes such as CTH (We plan to collaborate with the Sandia research associates on incorporation of the most promising indicators in the CTH applications code.). An extensive series of benchmark tests and comparison studies using different error indicators that include shape quality indicators will also be performed using the EPIC code. An important task in this part of the focused effort will be to investigate techniques for solving mesh aspect ratio degeneracy and the affect on solution quality and algorithm efficiency. Finally, we will continue and expand our work on mesh partitioning studies for parallel processing using domain decomposition on unstructured grids with TICAM and Sandia code modules. This work will include statistical studies of partitionings for representative adaptive grids obtained both with the 2:1 block refinement scheme in our CTH algorithms and also the fully adaptive moving grids obtained with the EPIC simulator.

9. Deliverables:

- Presentations at DoD HPC Users Group Conference and SC2000
- PET technical reports and journal articles detailing results of the project, testbed software, mesh quality strategies, new algorith ms developed, error indicator/adaptivity analysis and partitioning studies
- Support for implementation of selected adaption methods in DoD codes
- Software for the CSM testbed with supporting technical documentation and test application studies
- Visit to Vicksburg and briefing to ERDC MSRC on research program
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Focused Effort Title:** Discontinuous Galerkin Finite Elements and Adaptive Grids for DoD Problems

2. **Organization:** TICAM, University of Texas at Austin

4. **PI Names:** Prof. Graham Carey, Prof. Tinsley Oden

5. **E-Mail:** carey@cfdlab.ae.utexas.edu, oden@ticam.utexas.edu

6. **Telephone:** 512-471-4676, 512-471-3312

7. **Fax:** 512-232-3357, 512-471-8694

3. **Thematic Areas:** Scalable Computing Migration, HPC Performance Metrics/Tools

8. **Statement of Work:**

The purpose of this project is to promote and develop new advanced computational techniques with technology transfer to DoD Applications codes. The focus of this effort will involve the development, analysis, testing and implementation of new Discontinuous Galerkin techniques for finite element simulations. Such methods have recently become the center of interest for certain finite element applications in the research community. They appear particularly appealing for transient simulations of applications with shock –like structures and similar hyperbolic or near-hyperbolic problems of interest to DoD users. (In the DG schemes the continuity requirements across the interfaces between elements are enforced only weakly in the variational formulation rather than in the basis itself. This implies that the degrees of freedom can be local to the element and allows for local conservation and other properties to be enforced more strongly at the element level, with easier migration to higher degree elements. Stability and other properties may also be improved relative to other more conventional formulations.) These ideas will be investigated within the framework of unstructured grid approaches and adaptive grid technology that will enhance the accuracy and performance of CSM codes used by DoD researchers for damaged structures analysis. For applications such as blast calculations where there are strong shock layers and the standard schemes may be mesh sensitive near the blast layer this type of scheme is of interest. The incorporation of adaptive refinement of elements may also be easier from the standpoint of the underlying data structure permitting discontinuities and “hanging nodes”. This project also involves issues related to solution algorithms for these discontinuous Galerkin schemes, and compatibility with existing data structures in current DoD analysis codes. It also deals with problems related to module formulation and application programming interfaces for incorporation within existing and future DoD analysis codes to meet the DG adaptive mesh refinement (AMR) objective, support of related data structures, development of *a posteriori* error estimates and computable error indicators for this DG formulation.

The research and development work proposed below will build on the contributions of the previous year’s work which was designed to explore adaptive strategies for DoD codes based on established methodology. Specifically (i) we have established the feasibility of adding the adaptive capability to CSM legacy codes such as CTH and EPIC; (ii) we have made base case simulation studies using both application codes; (iii) we have performed

initial theoretical studies and interfaced a simple but representative error indicator to EPIC; (iv) we have made a test simulation with the indicator and local refinement; (v) we have begun design of a CSM testing c ode that will accelerate development and evaluation of new indicators, reliability of calculations and improved algorithms for CTH and similar DoD codes. An analysis and testing tool termed the "testbed" has been developed to accelerate testing of algorithms and error indicators, under the prior year's funding. This investment in the testbed is to be exploited in the work proposed here on Discontinuous Galerkin methodology, implementation issues and applications tests. Further details are listed in the ne xt section on R&D Tasks.

R&D Tasks: Research and Development work on DG methodology, algorithms and software implementation/testing. Specifically this will involve work on:

1. Investigation of DG formulations for analysis of hyperbolic and near -hyperbolic (including dissipation) problems such as those involved in Blast simulations of interest to DoD. Users.
2. Theoretical studies of the accuracy and stability of DG schemes for these problem classes.
3. Implementation of the DG method in the "Testbed" Framework for local adaptive simulations, developed under the prior year of funding.
4. Analysis of data structures and applications program interfaces for Migration of DG into DoD legacy and new codes.
5. Formulation and theoretical analysis of error indicators to gui de refinement and coarsening using DG.
6. Simulation and comparison studies for benchmark test cases and coordination of applications studies with DoD researchers.

9. Deliverables:

- Contributions to the PET CSM web page on DG methods, adaptive algorithms, t est problems, error analysis, etc.
- Journal articles detailing results of the project, new methodology, algorithm development, performance results and error indicator/adaptivity analysis
- Software and testing for CSM testbed with supporting technical documen tation
- Visit to Vicksburg and briefing to ERDC MSRC on research progress
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Focused Effort Title:** Algorithms for Error and Feature Indication in Interpolation and Approximation

2. **Organization:** TICAM, University of Texas at Austin

3. **Thematic Area:** Scalable Computing Migration

4. **PI Name:** Prof. Graham Carey, Prof. Tinsley Oden

5. **E-Mail:** carey@cfdlab.ae.utexas.edu, oden@ticam.utexas.edu

6. **Telephone:** 512-471-4676, 512-471-3312

7. **Fax:** 512-232-3357, 512-471-8694

8. **Statement of Work:**

The CSM TICAM members plan to provide algorithms and software for error or feature indicators that can be used in conjunction with the interpolation library (INLiB) routines provided by Dr. Bharat Soni, MSU. The TICAM CSM team members will also work on h,p and hp approaches and error indicators suitable for these classes of approximation. The h adaptive approaches will be applied in numerical tests on the "Testbed" software being developed in support of our other focussed effort activity. The CSM TICAM group will also work on software for projections between different grids including constrained projections for interfaces. The deliverables are a technical description of the interpolation bases, their approximation properties, the related algorithms and implementation together with supporting software modules. Dr. Carey will visit with Dr. Soni during the fall semester (probably at the Meshing Roundtable) to review progress.

9. **Deliverables:**

- Contribution to PET Annual Report
- Presentations for PET Mid-Year and Annual Reviews
- Contributions to PET CSM web page on capability enhancements, algorithms, test problems, and performance results
- PET technical reports, conference papers and journal articles detailing results of the project, expanded capabilities, new algorithm development, analysis, performance and application studies
- Software for INLiB package with supporting technical documentation
- Coordination visit with MSU researchers

1. **Core Support Area:** Environmental Quality Modeling and Simulation (EQM)
2. **Organization:** TICAM, University of Texas at Austin
3. **Lead:** Prof. Mary Wheeler
4. **E-Mail:** mfw@ticam.utexas.edu
5. **Telephone:** (512) 475-8625
6. **Fax:** (512) 471-8694
7. **Statement of Work:**

In this project, The University of Texas at Austin (UT-Austin) will support research and an on-site person in the EQM area. Technology transfer will occur through the on-site EQM personnel, the EQM web page, EQM success stories, activity reporting and user training. UT-Austin personnel will accomplish user outreach through frequent visits to user sites and contacts with users. UT-Austin personnel will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer.

Support for EQM codes includes the following:

1) Improved parallel performance of ADCIRC, CE-QUAL-ICM and CE-QUAL-ICM/TOXI. A version of CE-QUAL-ICM with persistent message passing will be developed, to improve the parallel scalability of this code. Also, better handling of the time-step computation within CE-QUAL-ICM will be addressed.
2) Parallel migration of UTPROJ-3D, as well as assistance in coupling of UTPROJ-3D with other EQM codes.
3) Provide assistance in migration of the new CH3D-Z code.
4) Improve the performance of the (CWO/EQM) codes POM and NAM-NPS and provide assistance in parallel migration as well as setup model run for DoD users.

8. **Deliverables:**

- Improved version of CE-QUAL-ICM (August 2000)
- Papers for DoD HPC Users Group Conference, SC2000, SIGGRAPH 2000, and PDSC Conference
- Workshop on Reactive Transport/Unstructured Grids
- Workshop on Multiphysics Applications
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- At least one technical report by on-site lead

1. **Focused Effort Title:** Improved Parallel Performance for Environmental Quality Models

2. **Organization:** TICAM, University of Texas at Austin

3. **Thematic Areas:** HPC Training and DoD User Productivity,
Scalable Computing Migration

4. **PI Names:** Prof. Mary F. Wheeler, Dr. Victor Parr

5. **E-Mail:** mfw@ticam.utexas.edu , parr@ticam.utexas.edu

6. **Telephone:** (512) 475-8625

7. **Fax:** (512) 471-8694

8. **Statement of Work:**

In parallelizing EQM codes, two of the main bottlenecks to achieving optimal parallel scalability are message passing and input/output. In this project, we will investigate the use of persistent and asynchronous message passing and the use of parallel I/O tools. As a test bed, these tools will be implemented within the parallelized water-quality model CE-QUAL-ICM, however the lessons learned here will benefit all parallel EQM codes. In particular, we will undertake the following tasks:

1) The message-passing interface in CE-QUAL-ICM will be rewritten. VAMPIR analysis of the message-passing in CE-QUAL-ICM showed that the current message-passing code must be optimized for improved scalability. The team has discussed the current design and has a well-defined plan. During the simulation the processors communicate concentrations, volumes, and a joint decision to compute the next timestep. Persistent message-passing will be used to reduce the overhead in communicating the concentrations. We have found a method to eliminate volumes information passing, and we have found an asynchronous approach to doing the timestep update. These three techniques will greatly improve CE-QUAL-ICM's parallel performance on all size problems.

2) CE-QUAL-ICM generates a tremendous amount of output. For example, to run the Chesapeake Bay scenarios 13 files per CPU are open at any given time. For large problems requiring on the order of 100 processors, the application must have 1300 files open simultaneously. We will investigate the use of MPI parallel I/O tools to write shared output files, including the tool MPI-Connect-I/O developed by the University of Tennessee PET team. This will reduce the total number of files in a 100 CPU run from 1300 to 805. Another benefit of this approach is that it eliminates the need for post-processing the local output files, a time-consuming task.

9. **Deliverables:**

- Rewrite of CE-QUAL-ICM message-passing and using the parallel tool VAMPIR to evaluate the parallel improvement (June 30, 2000)
- Implement MPI parallel I/O tools on all CE-QUAL-ICM output files (October 31, 2000)

- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Focused Effort Title:** A Full 2-D Parallel Implementation of CH3D-Z

2. **Organization:** TICAM, University of Texas at Austin

3. **Thematic Areas:** HPC Training and DoD User Productivity, Scalable Computing Migration

4. **PI Names:** Prof. Mary F. Wheeler, Prof. Clint Dawson

5. **E-Mail:** mfw@ticam.utexas.edu, clint@ticam.utexas.edu

6. **Telephone:** (512) 475-8625

7. **Fax:** (512) 471-8694

8. **Statement of Work:**

The CH3D-Z code is a widely used EQM hydrodynamics flow simulator, and is of high priority for efficient parallel migration. As a follow-on project of replacing the ADI solver in the CH3D-Z code, we propose a 2-D domain decomposition parallelization to improve the performance of the code. The approach that we will take is very similar to what we have used to successfully parallelize CE-QUAL-ICM and ADCIRC; i.e., a pre-processor will be developed which partitions the data among the processors, MPI calls will be added to the code itself for message-passing, and a post-processor will be used to gather the local information into global output files. However, there are some issues that are unique to CH3D-Z, which will need to be investigated. We will also investigate the use of OpenMP to enhance the performance of the code on a single processor or cluster of shared memory processors.

The modification made to this code will be transferable to other versions of the CH3D code including CH3D-SED and CH3D-COSED for sediment transport modeling. As part of this project, we will collaborate with the OSU PET team on migrating the new solver into other versions of the CH3D code.

9. **Deliverables:**

- Initial parallel version of parallel CH3D-Z (December 31, 2000)
- Fully tested version and user's guide (March 31, 2001)
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Focused Effort Title:** Interpolation and Projection Between Arbitrary Space/ Time Grids

2. **Organization:** TICAM, University of Texas at Austin

3. **Thematic Areas:** HPC Training and DoD User Productivity,
Scalable Computing Migration

4. **PI Names:** Prof. Mary F. Wheeler, Prof. Clint Dawson

5. **E-Mail:** mfw@ticam.utexas.edu, clint@ticam.utexas.edu

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8. **Statement of Work:**

In this project, we will collaborate with the MSU PET team in the development of methodology and software for interpolating and/or projecting quantities from one finite element grid to another. The particular application of interest is the coupling of hydrodynamic and environmental water quality models, however, the same problem arises when coupling groundwater flow and transport codes.

In these EQM applications, the flow and transport are often solved separately using different numerical methods and grids due to differences in time and length scales involved. For example, the flow grid usually needs to incorporate high resolution near land boundaries and should extend into the ocean to avoid spurious boundary effects. The transport code may only simulate transport over a small portion of the flow domain, and may use much coarser resolution. Therefore, for efficient coupling of flow and transport codes, it is critical to be able to take velocities and elevations from an arbitrary space/time flow domain, and interpolate or project them onto an arbitrary transport grid. Moreover, this must be done generally at every transport time step. Thus, this operation can be very costly if not implemented efficiently.

This project is a follow-on to our work last year on projection methods. Once velocities and elevations have been interpolated, they need to be further projected so as to satisfy the underlying conservation principles. Over the past year, we have developed a software package, UTPROJ, which computes conservative velocity fields on a given unstructured grid. The code has been interfaced with TABS-MDS for the purpose of testing the algorithms, and, at the moment, we are using the grid provided by TABS-MDS. In order for UTPROJ to be a truly useful tool for EQM users, however, we must have the more general interpolation capability described above.

Furthermore, while the current version of UTPROJ is robust, further work is needed to improve the parallel preconditioners in the code.

9. **Deliverables:**

- Version of UTPROJ with improved preconditioners (July 31, 2000)

- Demonstrate coupling of UTPROJ and CE-QUAL-ICM with an "arbitrary" hydrodynamics grid (January 31, 2001)
- Journal papers on projection methodology, and a related workshop on interpolation and projection between space-time grids (September 2000)
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Focused Effort Title:** Reactive Transport Schemes for Water Quality Modeling on Unstructured Grids

2. **Organization:** TICAM, University of Texas at Austin

3. **Thematic Areas:** HPC Training and DoD User Productivity, Scalable Computing Migration

4. **PI Names:** Prof. Mary F. Wheeler, Prof. Clint Dawson

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8. **Statement of Work:**

ERDC has a substantial on-going effort in water quality modeling, through such codes as CE-QUAL-ICM and CE-QUAL-ICM/Toxi. These codes contain very sophisticated aquatic chemistry, but use somewhat dated numerical methods for modeling advection, diffusion and reactions, and rely on the use of logically rectangular elements. We propose to investigate and develop conservative, higher-order accurate methods for advection and diffusion, suitable for any type of elements. The methodology to be investigated is based on the so-called discontinuous Galerkin (DG) methods, which have been developed by Wheeler, Dawson and their collaborators over the past few years. These methods are locally conservative, can be defined on any type of element (in fact the elements can be non-conforming), and allow for higher-order accuracy. They are especially useful for so-called h-p adaptivity, where one locally varies both the size of the element and the degree of the approximating polynomial. We will implement the methodology first within the current structure of the (parallel) CE-QUAL-ICM code, for comparison with the existing algorithms. We will also provide ERDC with a prototype three-dimensional advection-diffusion code on unstructured grids based on the DG methodology.

The discontinuous Galerkin methodology will also be investigated by Drs. Carey and Oden in a PET CSM focused effort on the modeling of shocks arising in impact problems. We will collaborate with our colleagues at UT Austin on the theory and implementation of DG methods for advection-dominated applications.

Another important issue that arises in these applications is in the area of time-splitting/time-stepping; i.e., within a given time step, how and in what order does one perform the advection, diffusion and reaction calculations? Generally, the nonlinear reactions are split from advection and diffusion, so as to avoid having to solve huge nonlinear systems of equations. But this approach becomes questionable when dealing with both equilibrium and kinetic reaction models. We will investigate, along with ERDC personnel, methods for dynamically coupling equilibrium chemistry models with transport/kinetic models. We have had some experience with these types of problems when dealing with bio- and geo-chemistry in groundwater. However, there are a number of issues with respect to accuracy, stability and robustness, which remain to be addressed.

9. Deliverables:

- Discontinuous Galerkin method implemented within existing CE -QUAL-ICM code, July 31, 2000.
- Prototype code on unstructured grids - advection-diffusion only, September 30, 2000
- Prototype code on unstructured grids - with chemical reactions, January 31, 2001
- Journal papers on discontinuous Galerkin methodology, and a related workshop on reactive transport (June 2000)
- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

1. **Focused Effort Title:** Parallel FEMWATER Visualization
2. **Organization:** Texas A&M University-Kingsville
3. **Thematic Area:** SciVis for Very Large Problems
4. **PI Name:** Prof. Thomas Lee McGehee
5. **E-Mail:** kftlm00@tamuk.edu
6. **Telephone:** (361) 593-3590
7. **Fax:** (361) 593-3068
8. **Statement of Work:**

Texas A&M University-Kingsville acquired sample FEMWATER datasets early this spring from the Groundwater Technical Support Group at the ERDC CHL. These files are stored on four DEC Alpha Servers at our university. The graduate student is working to perfect a front-end Fortran executable, which will load FEMWATER datasets into Ensight Gold 7.1. This work will be done by March 26, 2000. He is working his way through the tutorials to learn the modules. At the beginning of this funded period, he will begin training on GMS 3.0 at Texas A&M University – Kingsville. He will be learning the file structures and all visualization tools that are available in the model.

The next stage of research will take the team into visualizing FEMWATER datasets in Ensight Gold to develop flip-books and a video. This will require most of the students' summer time to develop several trial videos. Copies of the flipbooks and video will be sent to the Groundwater Modeling Technical Support Center for review and approval near the end of the summer. After the completion of the video presentation task, the graduate student will begin work on the tutorial. The team will try to determine the best use of the model for FEMWATER visualization and include these operations in the tutorial.

Dr. Thomas McGehee will travel to ERDC MSRC this summer to work with Jeffery Holland, Dave Richards, Barbara Donnell, and the research group with the Groundwater Technical Support Center. He will work on developing a strategy to model hydrogeologic phenomena , development of computational detail around surface hydraulic sources/sinks into a two - dimensional mesh, creation of surface and boundary layer TIN's, generation of the three - dimensional mesh, assignment of hydrogeologic properties and material types, and assignment of boundary conditions.

9. **Deliverables:**

- FEMWATER flipbooks and video fly-through
- FEMWATER tutorial to prepare images, flipbooks, and film loops in ENSIGHTS Gold 6.2
- FEMWATER models constructed on one or more of the above projects
- Generation of groundwater modeling mini-projects for graduate students from lessons learned at these sites

- Contribution to PET Annual Report
- Written progress reports in June and December 2000
- Presentations for PET Midyear and Annual Reviews
- Final Technical Report

ERDC MSRC PET YEAR FIVE EFFORTS

1. **Focused Effort Title:** Parallel FEMWATER Data Management

2. **Organization:** Texas A&M University-Kingsville

3. **Thematic Area:** Management and Interpretation of Large Data Sets

4. **PI Name:** Prof. Thomas Lee McGehee

5. **E-Mail:** kftlm00@tamuk.edu

6. **Telephone:** (361) 593-3590

7. **Fax:** (361) 593-3068

8. **Statement of Work:**

   Texas A&M University-Kingsville will continue to support two graduate students. Both have agreed to work on the EQM goals and objectives for this project as part of their master's thesis.

   Under the direction of the senior scientists at NCSA, University of Illinois at Urbana-Champaign and Texas A&M University-Kingsville, the students will continue their research on HDF5 (NSCA), GIS adaptation, and data visualization and reduction. The team at Texas A&M University-Kingsville will work closely with Mike Folk at NCSA and others at ERDC MSRC who have interest in the project.

   Drs. McGehee and McAdams will provide training on GMS to demonstrate the data techniques that we want these models to perform. At this point, we will require these students to analyze the capability of each module developed to perform the operation that GMS currently does in their respective models.

   These students will be expected to produce reports each month on their project and post these to our listserve. A working copy of the draft report comparing the two models will be in progress during this project period. We will provide EQM and the PET program access to these electronic reports to follow the progress of these projects.

9. **Deliverables:**

   - ERDC MSRC technical reports on the utility of HDF5 and other database management and GIS solutions in manipulating FEMWATER datasets
   - A general paper regarding data visualization and reduction from a supercomputer and GIS will be published in an appropriate journal or refereed publication
   - The team at Texas A&M University-Kingsville will test the tools developed by NCSA and prepare a report on these tests.
   - Contribution to PET Annual Report
   - Written progress reports in June and December 2000
   - Presentations for PET Midyear and Annual Reviews
   - Final Technical Report

Section 3: CONTACT INFORMATION

3.1 ACADEMIC POINTS OF CONTACT

- Academic Lead - Prof. Joe Thompson (ERC, Mississippi State University)
  - (601) 325-7299
  - joe@erc.msstate.edu

- HBCU/MI Lead - Prof. Willie Brown (Jackson State University)
  - (601) 968-6170
  - wbrown@jsums.edu

- Training Lead - Prof. Geoffrey Fox (Florida State University)
  - (850) 644-4587
  - gcf@cs.fsu.edu

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3.3 RELATED WEB ADDRESSES

ERDC Home Page: http://www.erdc.usace.army.mil/

ERDC MSRC Home Page: http://www.wes.hpc.mil/

ERDC MSRC Technical Reports: http://www.wes.hpc.mil/pet /tech_reports/available.htm

ERDC MSRC PET Training Schedule: http://www .wes.hpc.mil/training/training.htm

DoD HPCMP Home Page: http://www.hpcmo.hpc.mil/

DoD HPCMP PET Executive Committee: http://www.crpc.rice.edu/DODmod/index.html